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CFDRC

AN ADVANCED CAD TOOL FOR QUANTUM DEVICE SIMULATION

Progress Report

(May 1, 1999 - May 31, 1999)

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1. INTRODUCTION

This report describes the technical progress on the Office of Naval Research Project (Contract # N00014-99-M-0181) entitled "An advanced CAD tool for quantum device simulation". The current reporting period is May 1, 1999 through May 31, 1999.

2. TECHNICAL PROGRESS

The significant achievements during the first month of the project include finalizing a licensing agreement with Raytheon, coordinating a "universal" NEMO source code version to be shared by Raytheon, JPL, and CFDRC over the course of the SBIR and be the basis for the commercial quantum simulator package, and began preparations for implementation of AC small signal analysis. The accomplishments under the appropriate task are described below.

Task 1. Implement AC small signal analysis in an existing quantum simulator (NEMO) through S-parameter extraction:

Access to NEMO source code

The quantum simulator is based on the NEMO simulator. A development license is being finalized between Raytheon and CFDRC which gives CFDRC access to the latest NEMO source code and the right to develop and commercialize NEMO. Raytheon has also recognized JPL as an entity in which NEMO development can occur. Finally CFDRC is recognized by Raytheon as the caretaker of the "universal" source to be developed and marketed during the SBIR project.

Small signal AC analysis

Small signal AC analysis will be implemented in NEMO via a linear perturbative approach described by Fernando and Frensley [Fernando and Frensley, 1995]. A small sinusoidal potential is added to the diagonal of the Hamiltonian resulting in the generation of harmonics. Each harmonic corresponds to the order of response of the system due to the perturbing potential. The electric current resulting from the first and second order harmonics can be expressed as follows:

$$I = I_0 + \frac{v}{2}\left(ye^{i\omega t} + y^* e^{-i\omega t}\right) + \frac{a_{rect} v^2}{4} + \frac{v^2}{8}\left(a_{2\omega} e^{2i\omega t} + a^*_{2\omega} e^{-2i\omega t}\right) \qquad (1)$$

Here, I_0 is the DC current, v is the amplitude of the sinusoidal perturbation, y is the AC admittance, a_{rect} is the 2nd order rectification coefficient, and $a_{2\omega}$ is the 2nd order generation coefficient. The simulation of N orders of response requires the solution of N coupled Hamiltonians. The numerical implementation will leave

the order of harmonics under user control. On output the values of DC current, AC admittance as well as coefficients arising from all requested higher order harmonics will be provided. The AC admittance provides the input for SPICE models. The AC analysis will be implemented so that any of the NEMO bandstructure models may be employed. It will also be enhanced to include the generalized treatment of the open system boundaries [Klimeck et al., 1995; Lake et al., 1997] through guidance from Roger Lake at Raytheon.

<u>**Task 3. Task 3. Design architecture of 2D/ 3D, steady-state/transient, quantum/ hydrodynamic CAD tool:**</u>

A new architecture for the quantum simulator is being planned so the tool can be integrated into CFDRC's CAD architecture.

NEMO uses awk, C, FORTRAN, and FORTRAN 90 sources. Roughly 15% of NEMO is in FORTRAN 77/90 to enhance the calculation speed. Linear equations and eigenvalue problems in the code are solved using a freeware linear algebra package (LAPACK) accessed through Basic Linear Algebra Subprograms (BLAS).

A GUI or batch executable can be compiled from the source code. The batch or "non GUI" executable allows compiling the quantum simulator without the GUI. The GUI and batch source code are intermixed so that the GUI can call solver routines directly. The GUI uses a third party library for plotting routines. The "batch" version of NEMO operates from the command line and is faster and uses less memory than the GUI version.

Some of the redesign issues include:

- Decoupling the GUI from the solver routines in the source code.
- Using CFDRC's FOX libraries for GUI design instead of the Motif/3rd party plotting widget combination currently used by the tool.
- Comparing LAPACK solver performance with CFDRC numerical solver technology.
- Possibly reducing tool's dependence on mixed languages (C, FORTRAN, FORTRAN 90). Analyze performance of solvers using optimized C code.

3. DIFFICULTIES/PROBLEMS

There was a delay in the project progress due to the unavailability of the NEMO source. Since the source was not available, no progress could be made toward the implementation of the AC small signal analysis into NEMO source other than preparation through background reading of the approach that will be used. However, a developmental licensing agreement for NEMO source and theory has now been established with Raytheon. Also, the roles of Raytheon and JPL

under this SBIR have been established. The project will be on track at the time of the next reporting period.

4. PLANS FOR NEXT REPORTING PERIOD

- Establish common CVS repository of NEMO source
- CFDRC employee trained on NEMO source code and theory at JPL
- Implement AC small signal analysis into NEMO source
- Analyze NEMO source code architecture and make changes to improve portability between platforms, clearer separation between GUI directed activities and solver activities, specify UI using FOX libraries, and minimize use of mixed languages (C, FORTRAN 77, FORTRAN 90).

5. SCHEDULE

The project schedule is shown in Table 1.

Table 1. Work Schedule

TASK DESCRIPTION		Months After Receipt of Contract								
		1	2	3	4	5	6	7	8	9
Task 1.	Implement AC Small Signal Analysis									
Task 2.	Demonstration/Validation									
Task 3.	Design Architecture									
Task 4.	Final Report									
Task 5.	Solve Drift Diffusion (OPTION)									
Task 6.	Experimental Validation (OPTION)									

Work Completed   Work to be Done

6. REFERENCES

Fernando, C. L. and Frensley, W. R. (1995), "Intrinsic high-frequency characteristics of tunneling heterostructure devices," Phys. Rev. B, 52 (7), pp. 5092-5104.

Klimeck, G., Lake, R., Bowen, R. C., and Frensley, W. R. (1995b), "Quantum device simulation with a generalized tunneling formula," Appl. Phys. Lett., 67 (17), pp. 2539-2541.

Lake, R., Klimeck, G., Bowen, R. C., and Jovanovic, D. (1997), "Single and multiband modeling of quantum electron transport through layered semiconductor devices," J. App. Phys. 81 (2), pp. 7845-7869.